Microscopic multicluster description of neutron-halo nuclei with a stochastic variational method

K. Varga

Physics Department, Niigata University, Niigata 950–21, Japan

and

Institute of Nuclear Research of the Hungarian Academy of Sciences,
Debrecen, P. O. Box 51, H–4001, Hungary*

Y. Suzuki

Physics Department, Niigata University, Niigata 950–21, Japan

R. G. Lovas

Institute of Nuclear Research of the Hungarian Academy of Sciences,
Debrecen, P. O. Box 51, H–4001, Hungary

Abstract

To test a multicluster approach for halo nuclei, we give a unified description for the ground states of ^{6}He and ^{8}He in a model comprising an α cluster and single-neutron clusters. The intercluster wave function is taken a superposition of terms belonging to different arrangements, each defined by a set of Jacobi coordinates. Each term is then a superposition of products of gaussian functions of the individual Jacobi coordinates with different widths, projected to angular momenta $l = 0$ or 1. To avoid excessively large dimensions and "overcompleteness", stochastic methods were tested for selecting the gaussians spanning the basis. For ^{6}He, we were able to calculate ground-state energies that are virtully exact within the subspace defined by the arrangements and l values, and we found that preselected random sets of bases (with or without simulated annealing) yield excellent numerical convergence to this "exact" value with thoroughly truncated bases. For ^{8}He good energy convergence was achieved in a state space comprising three arrangements with all $l = 0$, and there are indications showing that the contributions of other subspaces are likely to be small. The ^{6}He and ^{8}He energies are reproduced by the same effective force very well, and the matter radii obtained are similar to those of other sophisticated calculations.

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*Permanent address.

1 Introduction

The discovery [1] of thick neutron clouds or "halos" in the surface of some light nuclei has led to a revival of interest in these nuclei, as is shown by numerous experimental and theoretical studies (see e.g. [2]). All candidates for halo structure are in the p-shell region, where systematics can be studied with the shell model, but the shell model runs into difficulties just in producing halos. To bring about a halo with a simple-minded enlargement of an harmonic-oscillator (h.o.) basis would in most cases require prohibitively large dimensions. If, alternatively, the single-particle orbits are chosen so as to exhibit the loosely-bound character of the halo [3], then the treatment of the centre-of-mass (c.m.) motion, of the Pauli principle and of continuum orbits pose extra problems.

The cluster-orbital shell model (COSM) [4] has solved these problems successfully, and, at least qualitatively, reproduced some known properties of the halo nuclei ^{6}He [4, 5], ^{8}He [4] and ^{11}Li [6]. But the COSM is not necessarily the ultimate model either. Even for the simplest case of ^{6}He, it is difficult to achieve convergence [5]. With the number of valence particles increased, this problem gets aggravated. On the other hand, the nuclei that have two halo nucleons are often "borromean": removal of one nucleon prompts a breakup of the rest by emission of another nucleon. It was shown that the three-body dynamics characteristic of such a system can be better described by inclusion of a core+n+n type three-cluster component [7].

The alternative models that focus just on the three-body aspects are the three-body models (see e.g. [8, 9]). None of the three-body calculations has, however, achieved unquestionable success. One problem is that the core–nucleon interaction, at least its off-shell behaviour, is not well-known. The accuracy of the treatment of antisymmetrization through Pauli projection (let alone through inclusion of a repulsive interaction [10]) depends crucially on the off-shell behaviour of the potential. Even if this treatment is satisfactory for the solution of the dynamical problem, there are extra three-cluster Pauli effects in the spectroscopic amplitudes characterizing the disintegration [11]. Moreover, it would be illusive to believe that cores like ^{9}Li are perfectly inert.

All these shortcomings call for fully microscopic treatments that preserve some elements of the few-body approaches as well. Although microscopic cluster models are general enough and their techniques are highly sophisticated [12, 13, 14], they have not been used too much to describe systems containing more than two clusters. It has been demonstrated recently for an α+p+n model of ^{6}Li that a microscopic approach, in which the treatment of the relative motion is comparable with the three-body approaches is feasible [15], and similar calculations for the ^{6}He–^{6}Li–^{6}Be isospin triplet have been published in another paper [16].

In the present paper we shall apply a multicluster approach to the ground state (g.s.) of the three-cluster system ^{6}He=α+n+n and of the five-cluster system ^{8}He=α+n+n+n+n. The present approach is similar to the previous one [15], except for some practical simplifications, which are compelling for ^{8}He, and, for consistency, are adopted for ^{6}He as well. The treatment of ^{6}He is a prerequisite of that of ^{8}He because some parameters are to be fitted to ^{6}He. The case of ^{6}He is used, at the same time, as a testing ground of the approximations introduced. We have solved the dynamical problems of these nuclei, hence obtaining the g.s. energies, and, to test the wave functions, we have calculated the rms point matter radii. Further applicaltions of our wave functions will be published in

a forthcoming paper.

The model is based on a linear variational method. The wave function is a superposition of cluster-model terms belonging to different sets of Jacobi coordinates or "arrangements", and the only parameters to be varied are the combination coefficients. Unlike before [15], we now choose purely central effective nucleon–nucleon interactions. This leads to a less realistic description of the relative motion, but it is more consistent with a purely s-state model of the α intrinsic motion [15]. In consistency with the use of a central force, we allow for fewer values of the intercluster orbital angular momenta. This is expected to be a fair approximation because the motion of two halo neutrons relative to each other, as well as of neutron pairs relative to a core, is dominated by s waves. Just as before, we expand the relative-motion functions in terms of gaussians of different widths. To counter the explosion of the basis size, we now have to introduce special truncation schemes for these expansions. We have examined systematic as well as stochastic methods for constructing the basis. As will be seen, the stochastic methods have proved more successful. It is owing to the stochastic variational procedure that this extremely versatile model is feasible for practical purposes.

The plan of the paper is as follows. In sect. 2 we outline the model used. In sect. 3 we introduce various basis truncation schemes and test them for ^{6}He. Sect. 4 comprises the results for ^{8}He, and sect. 5 contains a summary and some conclusions.

2 The multicluster model

The model we use is a generalization of the variational multiconfiguration multicluster approach outlined in ref. [15], and involves an α cluster and n single-neutron clusters. It employs a trial function, which is a sum over various cluster arrangements μ, each associated with a particular set of intercluster Jacobi coordinates $\{\boldsymbol{\rho}_1^\mu, ..., \boldsymbol{\rho}_n^\mu\}$. For α+n+n, there are two non-trivially different arrangements, viz. $\mu=(\alpha n)n$ and $\mu'=\alpha(nn)$, and the corresponding intercluster Jacobi coordinates are

$$\boldsymbol{\rho}_1 = \mathbf{r}_1 - \mathbf{r}_\alpha, \qquad \boldsymbol{\rho}_2 = \mathbf{r}_2 - \tfrac{1}{5}(4\mathbf{r}_\alpha + \mathbf{r}_1),$$
$$\boldsymbol{\rho}_1' = \mathbf{r}_2 - \mathbf{r}_1, \qquad \boldsymbol{\rho}_2' = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) - \mathbf{r}_\alpha, \qquad (1)$$

respectively, where $\mathbf{r}_\alpha$ is the position vector of the α c.m. and $\mathbf{r}_i$ are those of the extra neutrons. As is seen in fig. 1a, the Jacobi coordinates for $(\alpha n)n$ and $\alpha(nn)$ form a Y-shaped and a T-shaped pattern, respectively, and they will be referred to as such. For the system α+n+n+n there are four arrangements, $[(\alpha n)n]n$, $[\alpha(nn)]n$, $(\alpha n)(nn)$ and $\alpha[(nn)n]$, while for α+n+n+n+n there are nine: $\{[(\alpha n)n]n\}n$, $\{[\alpha(nn)]n\}n$, $[(\alpha n)(nn)]n$, $\{\alpha[(nn)n]\}n$, $[(\alpha n)n](nn)$, $[\alpha(nn)](nn)$, $(\alpha n)[(nn)n]$, $\alpha\{[(nn)n]n\}$ and $\alpha[(nn)(nn)]$. Fig. 1b shows a few of the five-cluster arrangements. As an illustration, here we give the Jacobi coordinates belonging to the TY-shaped arrangement $\{[\alpha(nn)]n\}n$:

$$\boldsymbol{\rho}_1 = \mathbf{r}_2 - \mathbf{r}_1, \qquad \boldsymbol{\rho}_2 = \tfrac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) - \mathbf{r}_\alpha,$$
$$\boldsymbol{\rho}_3 = \mathbf{r}_3 - \tfrac{1}{6}(4\mathbf{r}_\alpha + \mathbf{r}_1 + \mathbf{r}_2), \qquad \boldsymbol{\rho}_4 = \mathbf{r}_4 - \tfrac{1}{7}(4\mathbf{r}_\alpha + \mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3). \qquad (2)$$

The nucleon spins are coupled to S, and the orbital angular momenta l_i $(i = 1, ..., n)$, belonging to the Jacobi coordinates $\boldsymbol{\rho}_i$, are coupled to L. A term pertaining to arrange-

ment μ and angular momenta $[S, (l_1...l_n)L]JM$ can be written as

$$\Psi^{\mu}_{S,(l_1...l_n)L} = \mathcal{A}\left\{\left[\Phi_S \mathcal{X}^{\mu}_{(l_1...l_n)L}(\boldsymbol{\rho}^{\mu}_1, ..., \boldsymbol{\rho}^{\mu}_n)\right]_{JM}\right\}, \tag{3}$$

where $\mathcal{A}$ is the intercluster antisymmetrizer, Φ_{SM_S} is a vector-coupled product of the α intrinsic wave function Φ^{α} and the n neutron spin-isospin functions Φ^i, and $\mathcal{X}^{\mu}_{(l_1...l_n)L}$ is a vector-coupled product of the intercluster relative functions $\chi^{\mu}_{il_i m_i}(\boldsymbol{\rho}^{\mu}_i)$. The sequence of coupling is chosen so as to follow the pattern of the Jacobi coordinates. The intrinsic wave function of the g.s. of the α particle, Φ^{α}, is an h.o. Slater determinant divided by the 0s h.o. wave function describing the zero-point vibration of the α c.m. The h.o. size parameter $\nu = m\omega/2\hbar$ is determined by minimization of the α intrinsic hamiltonian. (The spatial factor of such a function is equal to a product of 0s h.o. functions of three intrinsic Jacobi coordinates.)

Representing each relative motion belonging to any single set of Jacobi coordinates by a complete set of functions, one can get a complete basis. The intercluster functions $\chi^{\mu}_{ilm}(\boldsymbol{\rho}^{\mu}_i)$ are, however, approximated by finite sums,

$$\chi^{\mu}_{ilm}(\boldsymbol{\rho}^{\mu}_i) = \sum_{k=1}^{N^{\mu}_i} C^{\mu}_{ikl}\Gamma^{\mu}_{iklm}(\boldsymbol{\rho}^{\mu}_i), \tag{4}$$

where Γ^{μ}_{iklm} are h.o. eigenfunctions of radial node number zero:

$$\Gamma^{\mu}_{iklm}(\boldsymbol{\rho}^{\mu}_i) = \left[\frac{2^{2l+7/2}(\nu^{\mu}_{ik})^{l+3/2}}{\sqrt{\pi}(2l+1)!!}\right]^{1/2}(\rho^{\mu}_i)^l \exp[-\nu^{\mu}_{ik}(\rho^{\mu}_i)^2]Y_{lm}(\hat{\boldsymbol{\rho}}^{\mu}_i). \tag{5}$$

The size parameters $\{\nu^{\mu}_{ik}, k = 1, ..., N^{\mu}_i\}$ should be chosen such that the functions Γ^{μ}_{iklm} adequately span the state space in the relative motion defined by the radial Jacobi coordinate ρ^{μ}_i. This can always be achieved since any well-behaved functions can be approximated with any prescribed precision by a combination of such functions. Because of the loosely-bound nature of these nuclei, more than one partial wave l_i may be needed for each relative motion, with a rather large N^{μ}_i (~ 10) for the radial motion in each partial wave, which entails an enormously large basis. Each set of Jacobi coordinates implies a particular asymptotic configuration, which involves few partial waves just when described in terms of these particular Jacobi coordinates. Therefore, the dimension may be reduced by combining the different arrangements:

$$\Psi_{(S,L)JM} = \sum_{\mu}\sum_{l_1...l_n}\Psi^{\mu}_{[S,(l_1...l_n)L]JM}, \tag{6}$$

where the lack of summations over S and L anticipates the choice of a purely central interaction.

The sets of Jacobi coordinates differ in what physical effects they emphasize. The Y-shaped and T-shaped branches of the diagrams of fig. 1 tend to magnify the correlation of the neutrons with a "core" and with each other, respectively. Thus, for ^{8}He the arrangement $\{[(\alpha n)n]n\}n$ is best suited to describing a shell-model-like configuration. The arrangements $[\alpha(nn)](nn)$ and $\alpha[(nn)(nn)]$ prefer two dineutron clusters, $(\alpha n)[(nn)n]$ and $\{\alpha[(nn)n]\}n$ favour the formation of a three-neutron cluster, $\alpha\{[(nn)n]n\}$ seems to

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accommodate a four-neutron cluster, while $\{[\alpha(nn)]n\}n$, $[(\alpha n)(nn)]n$ and $[(\alpha n)n](nn)$ are moulded to contain one dineutron and two neutrons moving around a core in a single-particle manner. It is *a priori* obvious that some of these configurations are very similar to each other, for instance, the last three arrangements only differ in what the core is. Thus it seems sufficient to include a few of these configurations. Even so, the basis sub-sets belonging to different arrangements do have large overlaps [15, 16], especially for small distances, which not only allows but, to avoid (numerical) overcompleteness, also necessitates truncations.

Both the angular momenta and the expansion of the radial functions are to be truncated. From among highly overlapping subspaces, we shall keep those with pure $l_i = 0$ because, for several clusters, the calculation of the matrix elements with non-zero l_i is very lengthy. To introduce a truncation of the expansion of the radial function $\mathcal{X}$, we need to substitute (4) into $\mathcal{X}$ involved in eq. (3):

$$\mathcal{X}^{\mu}_{(l_1...l_n)L\Lambda} = \sum_{K} D^{\mu}_{K,l_1...l_n} \left[\Gamma^{\mu}_{1k_1l_1}...\Gamma^{\mu}_{nk_nl_n} \right]_{L\Lambda}, \tag{7}$$

where $K \equiv \{k_1...k_n\}$, $D^{\mu}_{K,l_1...l_n} = C^{\mu}_{1k_1l_1}...C^{\mu}_{nk_nl_n}$, and the summation over K may be truncated such that it will no longer be equivalent to a sequence of summations over $k_1,...,k_n$.

The only variational parameters in the model are the coefficients $D^{\mu}_{K,l_1...l_n}$. Since ν^{μ}_{ik} are not varied, the bases will be somewhat redundant in the sense that there will exist smaller bases that would produce the same accuracy. To keep the variational method linear is, however, advantageous because the solution is reduced to a diagonalization over a non-orthogonal basis, and the method is founded on a genuine minimum principle. This implies that any estimate for any bound-state energy gives an upper bound, and the energies are lowered monotonously as the basis is extended. Moreover, if the basis is extended so that, in a limiting case, it fully spans a well-defined subspace of the state space, the energies will converge to the exact energies in that subspace. In the foregoing applications whole sets of variational calculations will be performed with stepwise extensions of the basis to make estimates for such "exact" energies by producing numerical convergence.

We chose the central effective interaction introduced by Thompson, LeMere and Tang [17], which has the form

$$V(i,j) = \left[V_R(r_{ij}) + \tfrac{1}{2}(1 + P^{\sigma}_{ij})V_t(r_{ij}) + \tfrac{1}{2}(1 - P^{\sigma}_{ij})V_s(r_{ij}) \right] \tfrac{1}{2} \left[u + (2 - u)P^{r}_{ij} \right], \tag{8}$$

where $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$, P^{σ}_{ij}, P^{r}_{ij} are the spin- and space-exchange operators, and $V(r_{ij})$ are of gaussian shape, and we neglected the Coulomb force, which would just shift the energy scale. This interaction reproduces, at least qualitatively, the most important low-energy nucleon–nucleon phase shifts, which implies that it does not bind the dineutron. On the other hand, by tuning the exchange parameter u, we can make the α+nucleon system comply with the borromean character of ^{6}He. The parameter u can be adjusted so as to reproduce the $p_{3/2}$ α+n phase shift and the ^{6}He binding energy E with respect to the three-body breakup threshold simultaneously, with reasonable accuracy. Without having a spin–orbit force, this is the best one can do. Since in ^{8}He the $p_{3/2}$ shell can accommodate all valence neutrons, this prescription is expected to cause little error. We chose u=1.14, which produces $E = -1.016$ MeV, while the experimental value is -0.975 MeV. The α

size parameter, rms point matter radius and energy implied by this force are $\nu = 0.303$ fm^{-2}, 1.363 fm and $E_\alpha = -25.581$ MeV, respectively.

The matrix elements involving the basis functions are expressed as integral transforms of matrix elements of Slater determinants, of shifted Gaussians, projected to total angular momentum JM. The technique applied is similar to that used in our earlier work [15].

3   Description of ^{6}He

In the description of a bound-state three-cluster system, like ^{6}He, the use of a large enough basis poses no problem. For the g.s. of ^{6}He, a central force renders the quantum numbers to pure $S = L = 0$ and $l_1 = l_2$. Appreciable contributions only come from the subspace defined by the T-shaped arrangement with $(l_1, l_2) = (0, 0)$ ("T$_{00}$ subspace") and by the Y$_{00}$ and Y$_{11}$ subspaces defined analogously. Radial bases of the types of eq. (5) with parameters

$$(\nu_{ik_i}^\mu)^{-1/2} = 0.7 \times 1.4^{k_i} \text{ fm} \qquad (k_i = 1, ..., 10; \ i = 1, 2) \qquad (9)$$

yield energies that are virtually exact within the model space defined by the arrangement(s) and value(s) of (l_1, l_2) adopted. In table 1 we give these energies along with the corresponding rms point matter radii for the three subspaces T$_{00}$, Y$_{00}$ and Y$_{11}$ and their unions.

The energies obtained in the individual subspaces are very close to each other, which shows that they are almost equally important, and yet, when they are combined, the binding gets stronger moderately. This behaviour is typical of strongly overlapping subspaces [20, 15, 16]. Although, as can be inferred from the table, none of the subspaces is large enough by itself, the combination {T$_{00}$,Y$_{11}$} does look like that. The fact that the energy produced by state space {T$_{00}$,Y$_{11}$} is hardly pushed down by inclusion of Y$_{00}$ (with the radius unchanged) indicates that the "full" wave function generated in the space {T$_{00}$,Y$_{00}$,Y$_{11}$} is in fact almost entirely contained in subspace {T$_{00}$,Y$_{11}$}.

The observed overlap between the subspaces suggests that the basis is largely redundant. It would be obviously desirable to reduce its dimension N by pinpointing redundant elements and dropping them. This is, however, not a trivial task because the overlaps of each particular element with all others are diverse. In the following we shall test various tactics of omitting elements and choosing elements so as to produce less redundant bases. We should emphasize that, even when the dimension is large (e.g., 300), the bulk of the computing time is spent on the computation of the matrix elements rather than on the diagonalization. Therefore, unlike in an earlier work on basis optimization [21], our aim is to reduce the number of matrix elements to be computed, and to this end, we are willing to make more diagonalizations.

The basis of each subspace defined by eq. (9) can be depicted in a $(b_1, b_2) = ((\nu_1^\mu)^{-1/2}, (\nu_2^\mu)^{-1/2})$ sheet as is shown in fig. 2a. We see that in each subspace for each Jacobi coordinate each function Γ occurs 10 times while the ν for the other Jacobi coordinate runs over all values. It is thus natural to ask whether one could get a satisfactory basis by a straightforward "thinning". Restricting ourselves to the T$_{00}$ space, we discarded half of the basis elements in a chessboard-like pattern shown by the open circles in fig. 2a (i.e. we kept $\{\Gamma_{1k_1l_1}^\mu, k_1 = 2, 4, ..., 10\}$ for k_2 odd and $\{\Gamma_{1k_1l_1}^\mu, k_1 = 1, 3, ..., 9\}$ for k_2 even). We obtained $E = -0.312$ MeV, which implies too much loss (0.083 MeV) of binding energy.

Alternatively, one may set up the basis with a stochastic method. First we present calculations with randomly chosen subsets of the basis elements defined by eq. (9), as exemplified by fig. 2b. Fig. 3 shows the energy versus dimension curves, $E(N)$, with three sets of T_{00} bases constructed by stepwise inclusion of such elements in fully random sequences. We see that the convergence is not too fast; by a 50% truncation, we may lose 200 keV of binding.

Given the above results, it is interesting to see whether we can gain anything from a continuously random basis. While in the previous attempt the labels, which are natural numbers, were picked randomly, now the ν values themselves, i.e. two *real* random numbers were generated independently. In our procedure the values of both ν were limited by imposing

$$1 \text{ fm} \leq \nu^{-1/2} \leq 10 \text{ fm}. \tag{10}$$

The bases generated in this way have proved excessively redundant. However, since the pool of basis states is infinitely large, it is reasonable to introduce some preselection. With this idea in mind, we introduced an admission procedure for extending the basis. Since any extension of the basis lowers the energy, the performance of a basis element can be judged by the energy improvement it causes. This obviously depends on the basis set in the previous step. At every step we tried 10 fully random basis states by adding one at one time in the basis constructed in the previous step, and admitted only the one that produced the lowest energy. A $((\nu_{1k_1}^{\mu})^{-1/2}, (\nu_{2k_2}^{\mu})^{-1/2})$ set obtained by such sequential random augmentations of the T_{00} basis is dispalyed in fig. 2c, and the results of three such sets of calculations are shown in fig. 4. All three sets converge rapidly. At dimensions 30 and 50 the energies are $-0.367, -0.380, -0.376$ MeV and $-0.393, -0.395, -0.394$ MeV, respectively, while the corresponding radii are 2.403, 2.442, 2.458 fm and 2.478, 2.467, 2.474 fm, respectively. Accepting an accuracy of, say 20–30 keV, we can say that, with such a random basis, a dimension of $\sim$30–40 for a single subspace is adequate. The reduction of the dimension with respect to the discrete case is obviously due to the selective sampling.

This method is comparable with stochastic basis selections that avoid full re-diagonalization at every step. Following ref. [21], we repeated the above procedure by replacing the full diagonalizations with those of 2×2 matrices formed by the model g.s. obtained in the previous step and the state to be tested. As is seen in fig. 5, this procedure converges to the wrong value, while the same bases with full diagonalizations throughout yield a convergence almost as good as that resulting from the selection based on repeated full diagonalizations. Thus, whereas the limiting energy obtained by sequential 2×2 diagonalizations is useless, the resulting basis is quite good. For problems in which the the diagonalization takes a higher proportion of the computing time, this procedure is recommendable as a method for basis construction, but one $N \times N$ diagonalization in the end is unavoidable.

When the three subspaces are combined, the random selection with full re-diagonalizations results in fig. 6. Three of the four curves were calculated by choosing 40, 20 and 20 basis elements from the subspaces consecutively, with three different sequences of the subspaces. It is seen that, while in the first subspace the convergence needs almost 40 elements, in the others it suffices to take substantially fewer. By subtracting the lengths, along which the curves are practically horizontal, we see that the fastest convergence could be attained by starting with subspace Y_{11}, which yields the deepest binding in a

single-subspace model (cf. table 1). In calculating the forth curve, the channel of each basis element was also chosen randomly. The initial section of this convergence curve is substantially steeper than the others, but, as we see in fig. 6, this is not a gain if we prescribe an accuracy of 20–30 keV. With the random sequence of channels a 20 keV accuracy is produced by dimension 45 ($E = -0.997$ MeV).

We have seen that a randomization with preselection may reduce the required dimension appreciably, but, in general, a random selection does not produce the optimum. It is possible that one can get a basis that is closer to the optimum by including all those and only those random elements that surpass a certain *preset* utility level. Utility is not an abstract quality; it should be understood with respect to the basis generated in the previous step. This level can thus be defined as a minimum energy improvement ε required of the inclusion of a would-be basis state. When the admittance is decided by a utility test, the convergence is automatically signalled by insistent failure to find further elements that pass the test.

In a pure T_{00} model the utility test with $\varepsilon = 0.005$ MeV did not improve the convergence, but in fig. 2d we still show such a basis. This apparently differs from the preselected random basis in two respects: it does not contain highly overlapping pairs of basis states and it contains fewer elements with both $\nu^{-1/2}$ small. In the full model this method looks definitely superior. In three runs, all with the sequence $\{T_{00}, Y_{00}, Y_{11}\}$, the energies and radii have converged to -0.999, -0.997, -0.998 MeV, and 2.429, 2.422 and 2.427 fm, at dimensions 45, 59, 47, respectively. When no basis element was found in a subspace to pass the utility test out of 10 consecutive attempts, the procedure was continued with the next subspace. In the last subspace, however, the calculations were only terminated when no basis element was found to fulfil the quality criterium after 100 attempts. The resulting energy and radius as a function of the dimension are shown in fig. 7. With $\varepsilon = 0.01$ MeV the energy deteriorated by a mere $\sim$20 keV (it converged to -0.986, -0.984, -0.969 MeV at $N = 48$, 39, 46, respectively), with a slightly larger scatter in the radii.

Although the energy deepens monotonously and the rate of deepening is mostly found to decrease with the basis increased, there is no theorem on the latter. For this reason, due caution should be excercised to avoid declaring convergence prematurely. In view of this, we modified the method as follows. After $\mathcal{N} = 10$ attempts failing to reach the utility level, we skipped the test once, i.e. we admitted a basis element that does not pass it. Such a procedure is called "simulated annealing" [22]. The random search for new elements was stopped after $10\mathcal{N} = 100$ consecutive failures to satisfy the utility criterium. With simulated annealing and parameter $\varepsilon = 0.01$ MeV the energy curves converged to -0.993, -0.996, -0.992 MeV at dimensions 59, 57 and 66, respectively. Thus the simulated annealing makes the method less economical, but it does make the procedure that involves utility tests safer.

Since the energy convergence attainable is not precise in a mathematical sense, one should check the quality of convergence for the wave function as well. The overall convergence can be judged from the fluctuations of the radius, which are acceptable for bases about to produce energy convergence (see figs. 4b and 7b). The critical domain of the nucleus is, however, the halo region, which may be extensive without contributing too much to the binding. For example, β-decay observables seem to be affected by the precise shape of the fall-off of the halo beyond 13 fm [23]. We tested the wave function through examining, in the T_{00} model, the two-variable function obtained by projecting out, from the

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wave function $\Psi^{\mathrm{T}}_{[0,(00)0]00}$, the α intrinsic motion and the $(l_1 l_2) = (00)$ angular component of the relative motions:

$$g(R_1, R_2) = R_1 R_2 \int d\hat{\mathbf{R}}_1 Y_{00}^*(\hat{\mathbf{R}}_1) \int d\hat{\mathbf{R}}_2 Y_{00}^*(\hat{\mathbf{R}}_2) \langle \mathcal{A}\{\Phi_0 \delta(\mathbf{R}_1 - \boldsymbol{\rho}_1)\delta(\mathbf{R}_2 - \boldsymbol{\rho}_2)\} | \Psi^{\mathrm{T}}_{[0,(00)0]00} \rangle.$$
(11)

This is in fact a spectroscopic amplitude. We examined the effect of including, in the basis, elements that emphasize the surface region. Starting with the 100-dimensional basis reported on in table 1, we included 10 more elements, resulting in a change of -0.00024 MeV and $+0.0027$ fm in the energy and radius, respectively. Meanwhile, the norm square of $g(R_1, R_2)$ changed from $s = 1.3570$ to 1.3568, and the change of $g(R_1, R_2)$ is very small accordingly. At the limit $R_1 = R_2 = 15$ fm, where $g(R_1, R_2)$ is 100 times smaller than its peak value, the change is 20%, and rapidly decreases with any of R_i smaller. Therefore, an integral over any of the two variables, like the function that enters into the description of β decay [23], carries a much smaller error. Thus the error found seems insignificant even for the halo properties. A random basis constructed with utility tests ($\varepsilon = 0.005$ MeV) and simulated annealing converges at $N = 36$, to yield an 0.008 MeV loss of binding and a -0.001 fm decrease of the radius (with respect to the 100-dimensional case) and $s = 1.3596$. The departure in $g(R_1, R_2)$ for large R values is, however, smaller than in the previous comparison, obviously because the difference between these two bases is not enhanced artificially in the asymptotic region. The slightly larger difference in s is due to a difference in $g(R_1, R_2)$ spread over a larger domain of (R_1, R_2). Thus we can claim that the basis reduction does not hit the asymptotic region more than any other region, and the method is as reliable in predicting the halo properties as any other properties.

To sum up, we have demonstrated that, by constructing the basis with stochastic sampling, the dimension required for an accuracy of 20–30 keV can be safely reduced by a factor of 5–6. We note that all results with random bases presented in this section have been corroborated by at least three different samplings. When there are more clusters, the basis is expected to be even more redundant, and an even larger reduction can probably be achieved. At the same time, however, there is more chance to be bogged down in flat areas, thus utility testing should always be accompanied with simulated annealing.

4   Description of ^{8}He

Since in the $\alpha+n+n+n+n$ model considered there are four Jacobi coordinates, it is beyond our means to construct a basis with a prescription like eq. (9) even in a single arrangement. (Then the dimension would be 10^4.) The experience with ^{6}He suggests, however, that, if numerical convergence can be reached with a random basis, then there is good hope that the limiting energy and wave function are approximately equal to the exact energy and wave function of the model problem. Moreover, it is easy to ascertain that this is so by examining whether different random bases converge to the same energy.

Fig. 8 shows that calculations with (preselected) random bases limited by eq. (10) converge rather slowly. The cause of this is to be found in that the domain of the four-dimensional "ν-space" included according to eq. (10) is rather large in comparison with the domain that gives rise to net attraction between the five clusters. By squeezing the limits in eq. (10), the convergence can only be speeded up for small dimensions because the outer

regions of this volume also contribute to the binding appreciably through interference in a configuration mixing. Therefore, we kept eq. (10) as it is.

Fortunately, however, the convergence can be speeded up by utility-tested basis states more radically than for ^{6}He. In the example of fig. 8, in subspace $\{[\alpha(nn)]n\}n$ with all orbital angular momenta zero, a preselected random basis leads to an apparent energy convergence at $E = -2.970$ MeV (measured from the $\alpha+n+n+n+n$ five-body breakup threshold) at dimension $N = 300$. Almost the same energy, $E = -2.961$ MeV, can be reached by utility testing of quality parameter $\varepsilon = 0.005$ MeV, with a simulated annealing of $\mathcal{N} = 10$, at dimension $N = 151$. Therefore, we adopt this prescription as the standard procedure. The energy is accepted as converged when failure to pass the test is detected for the 100th time consecutively. In multiconfiguration calculations we limited the dimension for each subspace to 120, which was either enough to attain convergence in the above sense or was very close to convergence. In the latter case it was left to the configurations to be included afterwards to make up for this slight omission as far as this is within their scope. We checked all convergence in all cases by at least one more independent set of calculations, and adopted the lower energy as the calculated model energy. The agreement between such independent calculations has always been better than 30 keV in energy and 0.005 fm in radius.

A review of the results is given in table 2. In all configurations considered the neutron spins are coupled to zero pairwise; in setting up these pairs we followed the pattern of the Jacobi vectors. All orbital angular momenta are assumed to be zero except those belonging to $\{[(\alpha n)n]n\}n'$, which are coupled as $\{[(l_1, l_2)l_{12}, l_3]l_{12,3}, l_4\}L = \{[(1, 1)0, 0]0, 0\}0$. The configurations considered are chosen so that each qualitatively different arrangement be represented.

If all angular momenta were included in each arrangement, each arrangement would span a complete basis by itself. Therefore, a comparison of the single-configuration calculations can be interpreted as testing the performance of the single-angular-momentum ansatz in each arrangement. Alternatively, since each configuration may as well be viewed as exhibiting certain types of intercluster correlation, these calculations may be interpreted as exploring these correlations. The difference between the configurations is surprisingly small. The good energy of the shell-model-like configuration with pure $l = 0$ shows the enormous flexibility of this model; after all, in the pure shell model a purely $l = 0$ configuration would carry an excitation of $4\hbar\omega$! The fact that the $\alpha+(4n)$-like configuration $\alpha\{[(nn)n]n\}$ performs so moderately shows that, in the "all $l = 0$ limit", the neutrons are more closely co-ordinated with the α cluster than with each other. At first sight, it looks surprising that the two $\alpha+(2n)+(2n)$-like configurations do not work equally well; $\alpha[(nn)(nn)]$ is less satisfactory obviously because it is closer to an $\alpha+(4n)$-type configuration like $\alpha\{[(nn)n]n\}$. The arrangement $(\alpha n)[(nn)n]$ is a representative of $\alpha+(3n)+n$-like formations, and, not surprisingly, is energetically disfavoured with $l = 0$ for similar reasons. The $\alpha+(2n)+n+n$-like arrangement yields a deep binding, which suggests that a configuration with two closely co-ordinated and two loosely co-ordinated neutrons, which is consistent with a two-neutron halo, has a large weight. The best result is, however, furnished by the $\{[(\alpha n)n]n\}n'$ configuration, which is not entirely unexpected since it contains, as it were, the best single ^{6}He configuration, Y_{11}.

Some of the multiconfiguration calculations show that the single-configuration models leave some room for improvements. The component $\alpha\{[(nn)n]n\}$ does not seem to add very

much to the best single configuration with $l = 0$, but the combination of the two favoured configurations, $\{[\alpha(nn)]n\}n$ and $[\alpha(nn)](nn)$, do improve on the energy substantially. The third favoured $l = 0$ configuration, $\{[(\alpha n)n]n\}n$, in $\{[\alpha(nn)]n\}n+[\alpha(nn)](nn)+\{[(\alpha n)n]n\}n$ still has an appreciable effect. Pilot calculations show, however, that a forth configuration has no significant effect. In particular, although the configuration containing $l = 1$, $\{[(\alpha n)n]n\}n'$, is the best by itself, it scarcely deepens the binding when added to the superposition $\{[\alpha(nn)]n\}n+[\alpha(nn)](nn)+\{[(\alpha n)n]n\}n$. This statement lacks preciseness because the $l \neq 0$ ingredients make full-fledged computations of such types prohibitively slow. We managed to include 17 basis states of subspace $\{[(\alpha n)n]n\}n'$ and that improved the energy by a mere 0.0015 MeV.

It was shown in ref. [24] that it is possible to reproduce the energies of ^{6}Li and ^{8}Be in the cluster model with the same central force rather well, but ^{8}He is much more complicated than ^{8}Be. Now we see that, just as ^{6}He, the nucleus ^{8}He is somewhat overbound by the force chosen. By modifying the mixing parameter from $u = 1.14$ to 1.135, the binding of ^{6}He reduces to -0.940 MeV (with $r = 2.462$ fm), while the $\{[\alpha(nn)]n\}n+[\alpha(nn)](nn)+\{[(\alpha n)n]n\}n$ model gives -3.041 MeV (with $r = 2.272$ fm) for ^{8}He. A linear interpolation shows that the force that puts the energy of ^{6}He right yields -3.204 MeV for ^{8}He, which is in excellent agreement with experiment, indeed. It is also remarkable that, while the separation energy of ^{8}He changes significantly, there is virtually no change in the radius. This suggests that the energy change, and thus the energy itself, is smeared all over the single-particle degrees of freedom.

5   Conclusion

We have argued that a thorough understanding of neutron-halo nuclei calls for a microscopic multicluster approach. In this paper we have demonstrated that such an approach is feasible. For the time being, we have adopted a central nucleon–nucleon interaction and a pure h.o. configuration for the α particle, and described the g.s. of the α+n+n and the α+n+n+n+n systems. We formulated the problem in a model space consisting of a few arrangements of the α and single-neutron clusters moving with orbital angular momenta of 0 or 1 around each other. This assumption takes shape in well-defined model state spaces, and we wished to get nearly exact g.s. solutions in these spaces. Our approach uses a linear variational method, and the main technical problem was the construction of a basis that contains this "exact" solution.

These multicluster problems are few-body problems aggravated by the complications coming from the internal structure of α. The exact solution of a nuclear five-body problem is beyond the present-day technical limits, and a most successful model-free approximation to such problems applies stochastic techniques in the variational calculus combined with similar (Monte Carlo) integration techniques (see e.g. [25]). The method we have now introduced for multicluster problems only applies random sampling techniques at the level of the variational approach, viz. in constructing the trial function. This approach is still feasible because all matrix elements involved can be calculated analytically, even though they need substantial amount of computation after all.

Drawing on former results, for ^{6}He we adopted a three-component state space, and constructed a basis in a systematic way. Invariance of the results against amendments to

the basis has proven that the basis contains the "exact" g.s. to a good approximation. Having such an "exact" solution, we tested ideas of constructing smaller bases that still encompass the "exact" solution. It was found that step-by-step enlargements of the basis by qualified random elements can be used to construct smaller but almost as good bases. What qualifies a basis function is its contribution to the energy when added in the basis constructed in the previous step. We tried to select candidates for basis states both by comparing them with each other (i.e. we singled out the best among a few in every step) and with an absolute scale (i.e. we singled out all that contribute more than a preset value). Since the latter type of selection ("utility testing") might terminate itself too soon, we allowed temporary lapses in the rigour of admittance ("simulated annealing").

For ^{8}He the same stochastic methods of constructing compact bases converged, and different methods or different random sets led to the same limiting energies. We thus have good reason to believe that these limiting energies are in fact the "exact" energies. While for ^{6}He any of the methods works equally well, for ^{8}He the utility testing proved definitely superior. To describe ^{8}He, it seems to suffice to include a three-component state space, which is a superposition of an α+(2n)+n+n-type, an α+(2n)+(2n)-type and a shell-model-like arrangement.

In spite of the simplicity of the interaction used, we managed to reproduce the g.s. energies of ^{6}He and ^{8}He simultaneously with an accuracy of 100 keV, which is a remarkable success. Nevertheless, the calculated matter radii of both nuclei undershoot the most recent experimental data. This result is consistent with that of Csótó [16] for ^{6}He, who used non-central terms along with the same central force, and extended the state space accordingly. These radii may be accounted for by the α-particle ingredient being too small; for the α wave function involved in the multicluster model has the same size parameter as producing 1.363 fm for the radius of the free α particle, which is $\sim 8\%$ smaller than the empirical value. This and other physical implications of the model will be discussed in a forthcoming paper.

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Table 1: Energies and rms radii of ^{6}He in different model spaces

Subspace	T_{00}	Y_{00}	Y_{11}	$\{T_{00},Y_{00}\}$	$\{T_{00},Y_{11}\}$	$\{Y_{00},Y_{11}\}$	$\{T_{00},Y_{00},Y_{11}\}$	Experiment
E (MeV)	−0.395	−0.387	−0.435	−0.944	−1.015	−0.605	−1.016	−0.975
r (fm)	2.455	2.441	2.451	2.411	2.443	2.469	2.442	2.4 [a]

[a] 2.48±0.03, ref. [18]; 2.33±0.04, ref. [19].

Table 2: Energies and rms radii of ^{8}He in different model spaces

Subspace [a]	N	E (MeV) [b]	r (fm) [c]
$\{[(\alpha n)n]n\}n$	153	−2.509	2.341
$\{[(\alpha n)n]n\}n'$; $\{[(1,1)0,0]0,0\}0$	130	−3.033	2.322
$\{[\alpha(nn)]n\}n$	161	−2.961	2.305
$[\alpha(nn)](nn)$	163	−2.676	2.278
$\alpha[(nn)(nn)]$	176	−1.167	2.188
$(\alpha n)[(nn)n]$	220	unbound	
$\alpha\{[(nn)n]n\}$	157	−1.368	2.196
$\{[\alpha(nn)]n\}n+[\alpha(nn)](nn)$	211	−3.292	2.306
$\{[\alpha(nn)]n\}n+\alpha\{[(nn)n]n\}$	223	−3.027	2.225
$\{[\alpha(nn)]n\}n+[\alpha(nn)](nn)+\{[(\alpha n)n]n\}n$	303	−3.395	2.271
$\{[\alpha(nn)]n\}n+[\alpha(nn)](nn)+\alpha\{[(nn)n]n\}$	311	−3.321	2.317

[a] The neutron spins are coupled to 0 pairwise, and all orbital angular momenta are zero except those belonging to $\{[(\alpha n)n]n\}n'$, which are coupled as $\{[(l_1,l_2)l_{12},l_3]l_{12,3},l_4\}L = \{[(1,1)0,0]0,0\}0$.
[b] Experiment: −3.112 MeV
[c] Experiment: 2.52±0.03, ref. [18]; 2.49±0.04, ref. [19].

Figure 1: Schematic diagrams depicting all possible sets of Jacobi coordinates for ^{6}He (a) and some possible sets for ^{8}He (b). The α cluster and the neutrons are represented by large and small dots, respectively.

Figure 2: The basis elements of the subspace T_{00} represented by full or open circles in the $(b_1, b_2) = ((\nu_1^\mu)^{-1/2}, (\nu_2^\mu)^{-1/2})$ sheet. The basis of $(\nu_{ik_i}^\mu)^{-1/2} = 0.7 \times 1.4^{k_i}$ fm ($k_i = 1, ..., 10$; $i = 1, 2$) with the open circles omitted in the chessboard-like thinning (a); a random subset (full circles) of the previous basis (b); a random basis with preselection (c); a utility-tested basis (d). Note the logarithmic scale!

Figure 3: Random paths of energy convergence in the T_{00} subspace on the pool of discrete basis elements of $(\nu_{ik_i}^\mu)^{-1/2} = 0.7 \times 1.4^{k_i}$ fm ($k_i = 1, ..., 10$; $i = 1, 2$).

Figure 4: Convergence in the T_{00} subspace (horizontal line: exact value) with (preselected) random bases in energy (a) and in the rms point matter radius (b).

Figure 5: Convergence in the T_{00} subspace (horizontal line: exact value) with consecutive 2×2 diagonalizations (short dashes), with full diagonalizations on the same bases (long dashes) and with a random basis constructed with full diagonalizations (full line).

Figure 6: Energy convergence with (preselected) random bases in the $\{T_{00}, Y_{00}, Y_{11}\}$ space. The four curves differ in the sequence of subspaces switched on. Sequence T_{00}, Y_{00}, Y_{11}: short-dashed curve; sequence Y_{00}, Y_{11}, T_{00}: medium-dashed curve; sequence Y_{11}, T_{00}, Y_{00}: long-dashed curve; basis elements randomized between subspaces: full curve; horizontal line: exact value.

Figure 7: Convergence of energy (a) and rms radius (b) produced by three random sequences of bases constructed with utility tests of parameter $\varepsilon = 0.005$ MeV in the $\{T_{00}, Y_{00}, Y_{11}\}$ space. Horizontal line: exact value.

Figure 8: Convergence of the ^{8}He energy with a (preselected) random basis (dashed curve) and with a basis constructed with utility tests of $\varepsilon = 0.005$ MeV and $\mathcal{N} = 10$ (full curve) in the subspace $\{[\alpha(nn)]n\}n$ restricted by all orbital angular momenta set to zero.